LECTURE 7

DERIVATION OF DIFFERENCE APPROXIMATIONS USING UNDETERMINED COEFFICIENTS

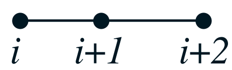
- All discrete approximations to derivatives are linear combinations of functional values at the nodes

$$f_i^{(p)} = \frac{a_\alpha f_\alpha + a_\beta f_\beta + \ldots + a_\lambda f_\lambda}{h^p} + E$$

- The total number of nodes used must be at least one greater than the order of differentiation p to achieve minimum accuracy $O(h)$.
- To obtain better accuracy, you must increase the number of nodes considered.
- For central difference approximations to even derivatives, a cancelation of truncation error terms leads to one order of accuracy improvement

Forward second order accurate approximation to the first derivative

- Develop a forward difference formula for $f_i^{(1)}$ which is $E = O(h)^2$ accurate
- First derivative with $O(h)$ accuracy $\Rightarrow$ the minimum number of nodes is 2
- First derivative with $O(h)^2$ accuracy $\Rightarrow$ need 3 nodes



- The first forward derivative can therefore be approximated to $O(h)^2$ as:

$$\left.\frac{df}{dx}\right|_{x = x_i} - E = \frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h}$$

- T.S. expansions about x_i are:

$$f_i = f_i$$

$$f_{i+1} = f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4$$

$$f_{i+2} = f_i + 2hf_i^{(1)} + 2h^2 f_i^{(2)} + \frac{4}{3}h^3 f_i^{(3)} + O(h)^4$$

- Substituting into our assumed form of $f_i^{(1)}$ and re-arranging

$$\frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h} = \frac{(\alpha_1 + \alpha_2 + \alpha_3)}{h} f_i$$

$$+ (\alpha_2 + 2\alpha_3) f_i^{(1)}$$

$$+ \left(\frac{\alpha_2}{2} + 2\alpha_3\right) h f_i^{(2)}$$

$$+ \left(\frac{1}{6}\alpha_2 + \frac{4}{3}\alpha_3\right) h^2 f_i^{(3)} + O(h)^3$$

- Desire $f_i^{(1)}$ and 2^{nd} order accuracy $\Rightarrow$ coefficient of $f_i^{(1)}$ must equal unity and coefficients of f_i and $f_i^{(2)}$ must vanish

$$\frac{\alpha_1 + \alpha_2 + \alpha_3}{h} = 0$$

$$(\alpha_2 + 2\alpha_3) = 1$$

$$\left(\frac{\alpha_2}{2} + 2\alpha_3\right) h = 0$$

- Solving these simultaneous equations

$$\alpha_1 = -\frac{3}{2}, \quad \alpha_2 = 2, \quad \alpha_3 = -\frac{1}{2}$$

- Thus the equation now becomes

$$\frac{-\frac{3}{2}f_i + 2f_{i+1} - \frac{1}{2}f_{i+2}}{h} = (0)f_i + (2-1)f_i^{(1)} + (0)f_i^{(2)} \qquad + \left(\frac{1}{6}\cdot 2 - \frac{4}{3}\cdot\frac{1}{2}\right)h^2 f_i^{(3)} + O(h)^3$$

$$\Rightarrow$$

$$f_i^{(1)} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{1}{3}h^2 f^{(3)} + O(h)^3$$

- The forward difference approximation of 2^{nd} order accuracy

$$\boldsymbol{f_i^{(1)} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + E \qquad \text{where} \quad E = \frac{1}{3}h^2 f_i^{(3)}}$$

Forward first order accurate approximation to the second derivative

- Derive the $O(h)$ forward difference approximations to $f_i^{(2)}$
- Second derivative $\Rightarrow$ 3 nodes for $O(h)$ accuracy

$$f_i^{(2)} - E = \frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h^2}$$

- Develop Taylor series expansions for f_i, f_{i+1} and f_{i+2}, substitute into expression and re-arrange:

$$\frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h^2} = \frac{(\alpha_1 + \alpha_2 + \alpha_3)}{h^2} f_i$$

$$+ \left(\frac{\alpha_2 + 2\alpha_3}{h}\right) f_i^{(1)}$$

$$+ \frac{1}{2}(\alpha_2 + 4\alpha_3) f_i^{(2)}$$

$$+ (\alpha_2 + 8\alpha_3)\frac{h}{6} f_i^{(3)} + O(h)^2$$

- In order to compute $f_i^{(2)}$ we must have:

$$\frac{1}{h^2}(\alpha_1 + \alpha_2 + \alpha_3) = 0$$

$$\frac{1}{h}(\alpha_2 + 2\alpha_3) = 0$$

$$\frac{1}{2}(\alpha_2 + 4\alpha_3) = 1$$

$$\Rightarrow$$

$$\alpha_1 = 1, \quad \alpha_2 = -2, \quad \alpha_3 = 1$$

- Therefore

$$\boldsymbol{f_i^{(2)} = \frac{1}{h^2}(f_{i+2} - 2f_{i+1} + f_i) + E \quad \text{where} \quad E = -hf_i^{(3)}}$$

Skewed fourth order accurate approximation to the second derivative

- Develop a fourth order accurate approximation to the second derivative at node i which involves nodes $i-1$, i and subsequent nodes to the right of node i

$f_i^{(2)}$ $\rightarrow$ requires 3 nodes for $O(h)$ accuracy

$\rightarrow$ requires 4 nodes for $O(h)^2$ accuracy

$\rightarrow$ requires 5 nodes for $O(h)^3$ accuracy

$\rightarrow$ requires 6 nodes for $O(h)^4$ accuracy

- Therefore we consider nodes

- $f_i^{(2)}$ is approximated as:

$$f_i^{(2)} - E = \frac{\alpha_1 f_{i-1} + \alpha_2 f_i + \alpha_3 f_{i+1} + \alpha_4 f_{i+2} + \alpha_5 f_{i+3} + \alpha_6 f_{i+4}}{h^2}$$

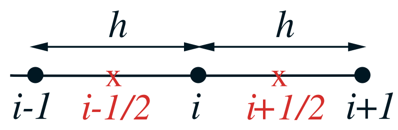
- Steps to solve for the unknown coefficients in the linear combination for $f_i^{(2)}$
  - Develop Taylor series expansions for f_{i-1} , f_{i+1} , f_{i+2} , f_{i+3} , f_{i+4}
  - Substitute and re-arrange to collect terms on equal derivatives
  - Generate equations by setting coefficients of $f_i^{(2)}$ to 1 and the remaining 5 leading coefficients to zero

NUMERICAL DIFFERENTIATION USING DIFFERENCE OPERATORS

Difference Operators

First order difference operators

- Consider the following full and intermediate nodes



- First order forward difference operator

$$\Delta f_i \equiv f_{i+1} - f_i$$

- First order backward difference operator

$$\nabla f_i \equiv f_i - f_{i-1}$$

- First order central difference operator defined using full node functional values

$$\delta f_i \equiv f_{i+1} - f_{i-1}$$

Notes

- Intermediate functional values are defined as

$$f_{i+\frac{1}{2}} = f\left(x_i + \frac{h}{2}\right)$$

- First order central difference operator defined using intermediate nodes

$$\delta f_i \equiv f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}$$

- The central difference operator is defined at an intermediate node as

$$\delta f_{i+\frac{1}{2}} \equiv f_{i+1} - f_i$$

- The ***order of the difference operator*** is related to the number of times that the operator is applied and not to the ***order of accuracy***

- Higher order difference operators $\rightarrow$ simply repeat operation as indicated by the operator

Second order forward difference operator

$$\Delta^2 f_i = \Delta(\Delta f_i)$$

$$= \Delta(f_{i+1} - f_i)$$

$$= \Delta f_{i+1} - \Delta f_i$$

$$= (f_{i+2} - f_{i+1}) - (f_{i+1} - f_i)$$

$$\boldsymbol{\Delta^2 f_i = f_{i+2} - 2f_{i+1} + f_i}$$

Third order backward difference operator

$$\nabla^3 f_i = \nabla^2(\nabla f_i)$$

$$= \nabla^2(f_i - f_{i-1})$$

$$= \nabla(\nabla f_i - \nabla f_{i-1})$$

$$= \nabla[(f_i - f_{i-1}) - (f_{i-1} - f_{i-2})]$$

$$= \nabla[f_i - 2f_{i-1} + f_{i-2}]$$

$$= \nabla f_i - 2\nabla f_{i-1} + \nabla f_{i-2}$$

$$= (f_i - f_{i-1}) - 2(f_{i-1} - f_{i-2}) + (f_{i-2} - f_{i-3})$$

$$\boldsymbol{\nabla^3 f_i = f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}}$$

Second order central difference operator

$$\delta^2 f_i = \delta(\delta f_i)$$

$$= \delta\left(f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}\right)$$

$$= \delta f_{i+\frac{1}{2}} - \delta f_{i-\frac{1}{2}}$$

$$= (f_{i+1} - f_i) - (f_i - f_{i-1})$$

$$\boldsymbol{\delta^2 f_i = f_{i+1} - 2f_i + f_{i-1}}$$

Second order mixed difference operator

- We can also apply different operators; e.g.

$$\nabla^{n-m}\Delta^m, \quad 1 \le m \le n$$

- Applying a first order forward difference operator and then a first order backward difference operator

$$\begin{aligned}\nabla\Delta f_i &= \Delta(\nabla f_i)\\ &= \Delta(f_i - f_{i-1})\\ &= \Delta f_i - \Delta f_{i-1}\\ &= (f_{i+1} - f_i) - (f_i - f_{i-1})\end{aligned}$$

$$\boldsymbol{\Delta\nabla f_i = f_{i+1} - 2f_i + f_{i-1}}$$

- We note that $\delta^2 = \Delta\nabla = \nabla\Delta$ and in general $\delta^{2m} = \nabla^m\Delta^m \rightarrow (2m)^{th}$ order central difference operator

Approximations to Differentiation Using Difference Operators

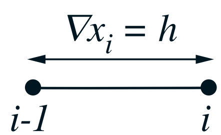
$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{\Delta f_i}{\Delta x_i}$$

$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{\nabla f_i}{\nabla x_i}$$

$$\left.\frac{df}{dx}\right|_{x_i} \cong \frac{\delta f_i}{\delta x_i}$$

First order backward difference operator approximation to the first derivative

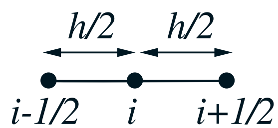
$$f_i^{(1)} \cong \frac{\nabla f_i}{\nabla x_i}$$



$$\boldsymbol{f_i^{(1)} \cong \frac{f_i - f_{i-1}}{h}}$$

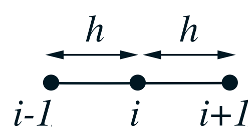
First order central difference operator approximation to the first derivative

$$f_i^{(1)} \cong \frac{\delta f_i}{\delta x_i}$$



$$\delta x_i = h$$

$$f_i^{(1)} \cong \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h}$$



$$\delta x_i = 2h$$

$$\boldsymbol{f_i^{(1)} \cong \frac{f_{i+1} - f_{i-1}}{2h}}$$

<u>Central difference approximation to the first derivative as an average of first order forward and backward difference approximations</u>

- We note that first order central difference approximations can also be derived as arithmetic averages of first order forward and backward difference approximations

$$f_i^{(1)} \cong \frac{1}{2}\left[\frac{\Delta f_i}{\Delta x_i} + \frac{\nabla f_i}{\nabla x_i}\right]$$

$$f_i^{(1)} \cong \frac{1}{2}\left[\frac{f_{i+1} - f_i}{h} + \frac{f_i - f_{i-1}}{h}\right]$$

$$\boldsymbol{f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2h}}$$

- This concept can be generalized to central approximations to higher order derivatives as well (see the next section)

General difference operator approximations to derivatives

- In general we can approximate derivatives using
  - Forward approximations

$$f_i^{(p)} \cong \frac{\Delta^p f_i}{h^p} + O(h)$$

  - Backward approximations

$$f_i^{(p)} \cong \frac{\nabla^p f_i}{h^p} + O(h)$$

  - Central approximations

$$f_i^{(p)} \cong \frac{\nabla^p f_{i+\frac{p}{2}} + \Delta^p f_{i-\frac{p}{2}}}{2h^p} + O(h)^2 \qquad p \text{ even}$$

$$f_i^{(p)} \cong \frac{\nabla^p f_{i+\frac{p-1}{2}} + \Delta^p f_{i-\frac{p-1}{2}}}{2h^p} + O(h)^2 \qquad p \text{ odd}$$

- A complete operator approach to central differencing can be developed. However this approach is somewhat artificial and overly complicated.